

chain nodes :

6 8 9 16 17 18 19 20 21 22 23 24 25 26 27 37 38 40 43 46 52 62

ring nodes :

1 2 3 4 5 10 11 12 13 14 15 47 48 49 54 55 56 57 58 59 72

chain bonds :

2-6 3-8 4-9 5-37 10-38 11-46 12-40 13-52 17-18 19-20 19-21 19-22 56-62

ring bonds :

1-2 1-5 3-4 3-72 4-72 10-11 11-12 13-14 14-15 14-47 15-49 47-48 48-49 54-55
54-57 55-56 55-59 57-58 58-59

exact/norm bonds :

1-2 1-5 2-6 3-8 3-4 3-72 4-9 4-72 5-37 10-11 10-38 11-12 11-46 12-40 13-14
13-52 14-15 14-47 15-49 17-18 19-20 19-21 19-22 47-48 48-49 54-55 54-57 55-56
55-59 56-62 57-58 58-59

G1:[*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8]

G2:Si,Hy,Ak,[*9]

G3:[*10-*11], [*12-*13], [*14-*15], [*16-*17]

Connectivity :

1:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:CLASS 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 37:CLASS 38:Atom 40:CLASS
43:Atom

46:CLASS 47:Atom 48:Atom 49:Atom 52:Atom 54:Atom 55:Atom 56:Atom 57:Atom

58:Atom 59:Atom 62:CLASS 72:Atom

Generic attributes :

6:

Number of Hetero Atoms : 2 or more

8:

Saturation : Unsaturated

9:

Saturation : Unsaturated

38:

Number of Hetero Atoms : 2 or more

43:

Saturation : Unsaturated

52:

Saturation : Unsaturated

Element Count :

Node 6: Limited

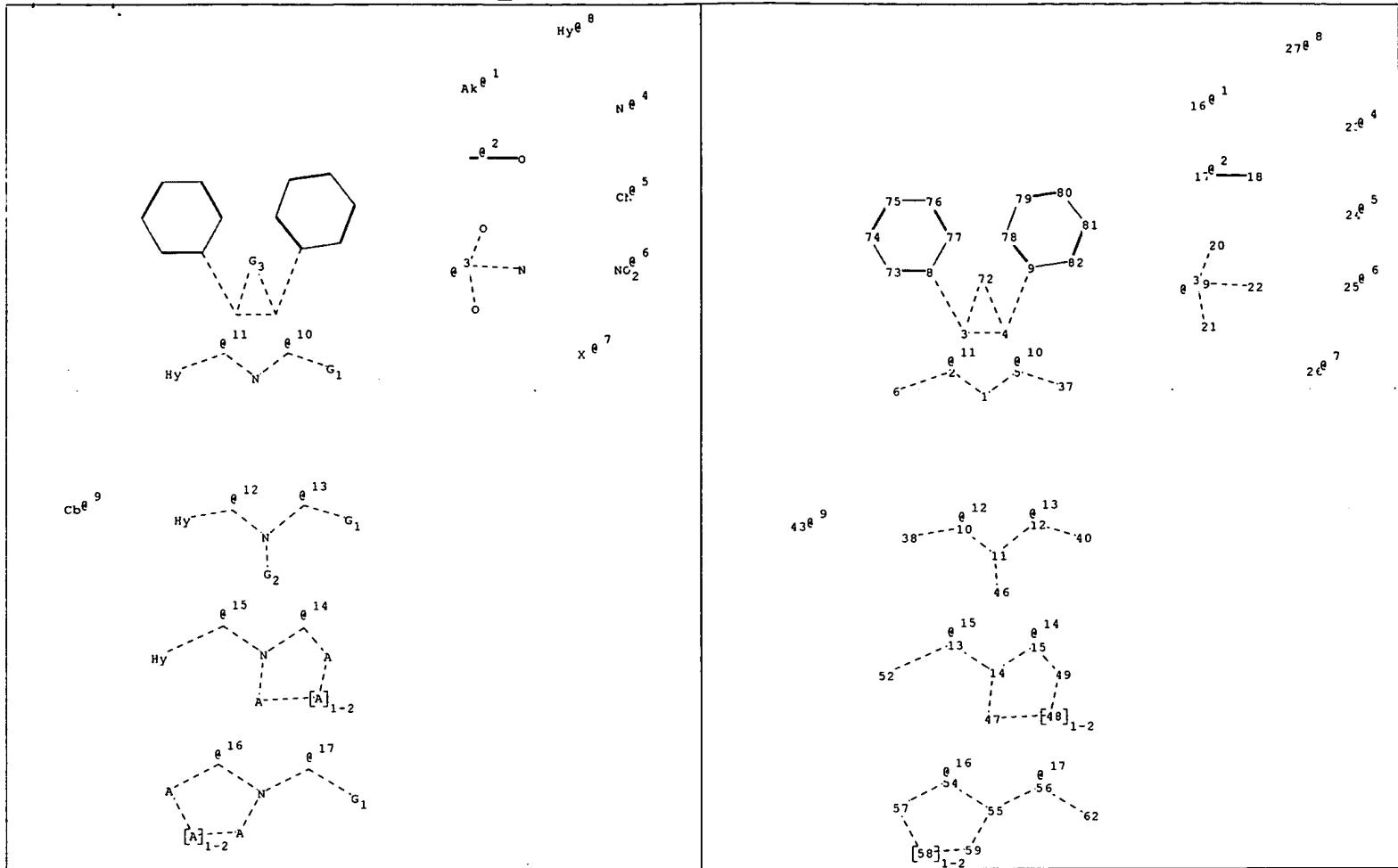
N,N1

Node 38: Limited

N,N1

Node 52: Limited

N,N1



chain nodes :

6 16 17 18 19 20 21 22 23 24 25 26 27 37 38 40 43 46 52 62

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 47 48 49 54 55 56 57 58 59 72 73
74 75 76 77 78 79 80 81 82

chain bonds :

2-6 3-8 4-9 5-37 10-38 11-46 12-40 13-52 17-18 19-20 19-21 19-22 56-62

ring bonds :

1-2 1-5 3-4 3-72 4-72 8-73 8-77 9-78 9-82 10-11 11-12 13-14 14-15 14-47
15-49 47-48 48-49 54-55 54-57 55-56 55-59 57-58 58-59 73-74 74-75 75-76 76-77
78-79 79-80 80-81 81-82

exact/norm bonds :

1-2 1-5 2-6 3-8 3-4 3-72 4-9 4-72 5-37 10-11 10-38 11-12 11-46 12-40 13-14
13-52 14-15 14-47 15-49 17-18 19-20 19-21 19-22 47-48 48-49 54-55 54-57 55-56
55-59 56-62 57-58 58-59

normalized bonds :

8-73 8-77 9-78 9-82 73-74 74-75 75-76 76-77 78-79 79-80 80-81 81-82

isolated ring systems :

containing 8 : 9 :

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8]

G2:Si,Hy,Ak,[*9]

G3:[*10-*11],[*12-*13],[*14-*15],[*16-*17]

Connectivity :

1:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:CLASS 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 37:CLASS 38:Atom 40:CLASS
43:Atom 46:CLASS 47:Atom 48:Atom 49:Atom 52:Atom 54:Atom 55:Atom 56:Atom 57:Atom
58:Atom 59:Atom 62:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom
79:Atom 80:Atom 81:Atom 82:Atom

Generic attributes :

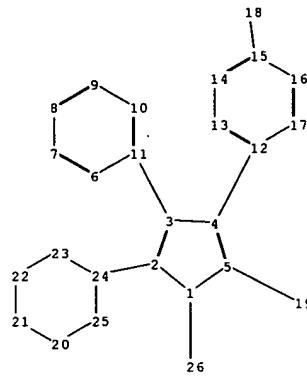
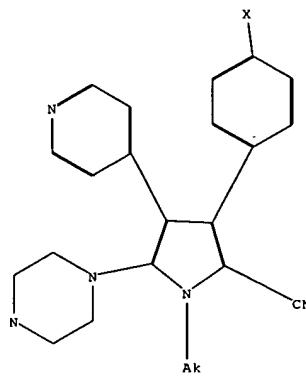
6:
Number of Hetero Atoms : 2 or more
38:
Number of Hetero Atoms : 2 or more
43:
Saturation : Unsaturated
52:
Saturation : Unsaturated

Element Count :

Node 6: Limited
N,N1

Node 38: Limited
N,N1

Node 52: Limited
N,N1



chain nodes :

18 19 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 20 21 22 23 24 25

chain bonds :

1-26 2-24 3-11 4-12 5-19 15-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15
15-16 16-17 20-21 20-25 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 1-26 2-3 2-24 3-4 4-5 20-21 20-25 21-22 22-23 23-24 24-25

exact bonds :

3-11 4-12 5-19 15-18

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS